ethyl 2-acetyloxypropanoate

2985-28-6 | DTXSID00277952

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.55e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.08e-01

Confidence level: 8.94e-01

Nearest Neighbors from the Training Set

Image not found
1,2-Phenylenediamine
Measured: 4.14e-01
Predicted: 8.53e-04

Image not found
Acetic acid, chloro-, 1-methylethyl ester
Measured: 2.69e-01
Predicted: 6.23

Image not found
Hexamethyleneimine
Measured: 7.74e-02
Predicted: 15.0

Image not found
4-Bromophenol
Measured: 4.10e-01
Predicted: 2.33e-02

Image not found
Benzene, (iodomethyl)-
Measured: 3.00e-01
Predicted: 1.97e-01